# Dereplication of Mammea neurophylla metabolites to isolate original 4-phenylcoumarins



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| Résumé en anglais | Mammea coumarins are isoprenylated 4-alkyl or 4-phenylcoumarins. Their distribution is limited to 3 Clusiaceae/Calophyllaceae genera. We recently reported on their presence in Mammea neurophylla bark extracts, where they exhibited anti-AGE properties associated with a prevention of the endothelial dysfunction. About 120 mammea coumarins were already described so, in order to focus further phytochemical analysis on original or bio-active compounds, we developed a methodology to facilitate the detection and identification of compounds of interest. Our aim was to develop a LC-DAD–ESI-MSn method for rapid, sensitive and simple analysis of the mammea coumarins in calophyllaceous/clusiaceous species. For that, full LC-DAD–MSn data were acquired from 11 4-phenylcoumarins previously isolated in our laboratory. Bark, leaves and fruits of M. neurophylla were then extracted with DCM using an ASE apparatus. Extracts were finally analyzed through LC-DAD–HRMSn and UV and MS profiles were compared to our database as well as literature data. Detected new compounds were isolated and their structures elucidated through 1H, 13C and 2D NMR analysis. Finally, 24 known mammea coumarins were dereplicated from bark, leaf and fruit DCM extracts of M. neurophylla and the structure of 4 unreported compounds could be predicted. In particular, the structures of mammea A/AA 9-hydroxyCycloF and mammea A/AB 9-hydroxyCycloF were confirmed after purification and extensive NMR analyses. By comparison of UV and mass fragmentation data from a small library of reference compounds, LC-DAD–HRMSn analysis of mammea coumarins in crude extracts allows the structure prediction of novel or bio-active compounds. This useful guiding-tool could be easily applied to other Clusiaceae/Calophyllaceae phytochemical analysis. |

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